



wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2020 – 01:58 am BST

PDB ID : 6C16
Title : Ubiquitin variant (UbV.Fbl10.1) bound to a human Skp1-Fbl11 fragment complex.
Authors : Manczyk, N.; Sicheri, F.
Deposited on : 2018-01-04
Resolution : 3.27 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

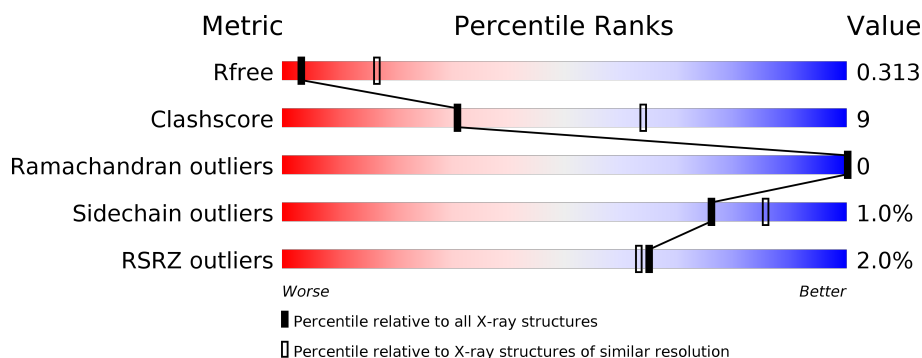
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	165	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>11%</div> <div>19%</div> </div> </div>
1	B	165	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>17%</div> <div>•</div> <div>16%</div> </div> </div>
2	C	47	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>6%</div> <div>26%</div> </div> </div>
2	F	47	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>•</div> <div>15%</div> </div> </div>
3	D	86	<div> <div></div> <div> <div>70%</div> <div>23%</div> <div>7%</div> </div> </div>
3	H	86	<div> <div>•</div> <div> <div>72%</div> <div>23%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3529 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	0	0
			909	583	146	175	5			
1	B	139	Total	C	N	O	S	0	0	0
			941	599	155	184	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P63208
A	0	ALA	-	expression tag	UNP P63208
B	-1	GLY	-	expression tag	UNP P63208
B	0	ALA	-	expression tag	UNP P63208

- Molecule 2 is a protein called Lysine-specific demethylase 2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	35	Total	C	N	O	S	0	0	0
			256	165	45	44	2			
2	F	40	Total	C	N	O	S	0	0	0
			255	164	43	43	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	886	GLY	-	expression tag	UNP Q9Y2K7
C	887	ALA	-	expression tag	UNP Q9Y2K7
F	886	GLY	-	expression tag	UNP Q9Y2K7
F	887	ALA	-	expression tag	UNP Q9Y2K7

- Molecule 3 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	80	Total	C	N	O	0	0	0
			559	353	97	109			
3	H	82	Total	C	N	O	S	0	0
			609	386	103	119	1		

There are 46 discrepancies between the modelled and reference sequences:

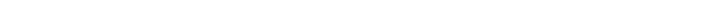
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP P0CG47
D	-1	SER	-	expression tag	UNP P0CG47
D	0	GLY	-	expression tag	UNP P0CG47
D	8	PHE	THR	engineered mutation	UNP P0CG47
D	9	ARG	GLY	engineered mutation	UNP P0CG47
D	10	ASP	LYS	engineered mutation	UNP P0CG47
D	11	ARG	-	insertion	UNP P0CG47
D	11a	LEU	-	insertion	UNP P0CG47
D	11b	ARG	-	insertion	UNP P0CG47
D	11c	ASN	-	insertion	UNP P0CG47
D	11e	LEU	-	insertion	UNP P0CG47
D	11f	PRO	-	insertion	UNP P0CG47
D	11g	GLN	-	insertion	UNP P0CG47
D	42	VAL	ARG	engineered mutation	UNP P0CG47
D	46	SER	ALA	engineered mutation	UNP P0CG47
D	47	ARG	GLY	engineered mutation	UNP P0CG47
D	49	ARG	GLN	engineered mutation	UNP P0CG47
D	68	ARG	HIS	engineered mutation	UNP P0CG47
D	72	VAL	ARG	engineered mutation	UNP P0CG47
D	73	PHE	LEU	engineered mutation	UNP P0CG47
D	74	GLY	ARG	engineered mutation	UNP P0CG47
D	75	ARG	GLY	engineered mutation	UNP P0CG47
D	76	ARG	GLY	engineered mutation	UNP P0CG47
H	-2	GLY	-	expression tag	UNP P0CG47
H	-1	SER	-	expression tag	UNP P0CG47
H	0	GLY	-	expression tag	UNP P0CG47
H	8	PHE	THR	engineered mutation	UNP P0CG47
H	9	ARG	GLY	engineered mutation	UNP P0CG47
H	10	ASP	LYS	engineered mutation	UNP P0CG47
H	11	ARG	-	insertion	UNP P0CG47
H	11a	LEU	-	insertion	UNP P0CG47
H	11b	ARG	-	insertion	UNP P0CG47
H	11c	ASN	-	insertion	UNP P0CG47
H	11e	LEU	-	insertion	UNP P0CG47
H	11f	PRO	-	insertion	UNP P0CG47

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Chain	Residue	Modelled	Actual	Comment	Reference
H	11g	GLN	-	insertion	UNP P0CG47
H	42	VAL	ARG	engineered mutation	UNP P0CG47
H	46	SER	ALA	engineered mutation	UNP P0CG47
H	47	ARG	GLY	engineered mutation	UNP P0CG47
H	49	ARG	GLN	engineered mutation	UNP P0CG47
H	68	ARG	HIS	engineered mutation	UNP P0CG47
H	72	VAL	ARG	engineered mutation	UNP P0CG47
H	73	PHE	LEU	engineered mutation	UNP P0CG47
H	74	GLY	ARG	engineered mutation	UNP P0CG47
H	75	ARG	GLY	engineered mutation	UNP P0CG47
H	76	ARG	GLY	engineered mutation	UNP P0CG47

GLY	SER	GLY	M1	F4	V5	K6	R11	T12	I13	D21	T22	I23	E24	N25	V26	K29	I30	Q31	D32	P37	Q41	V42	F45	R54	T66	L67	F73	GLY	ARG	ARG
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Chain H:  %



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.24Å 119.58Å 63.71Å 90.00° 98.45° 90.00°	Depositor
Resolution (Å)	19.82 – 3.27 19.82 – 3.27	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.82-3.27) 98.7 (19.82-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.29Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.260 , 0.317 0.257 , 0.313	Depositor DCC
R_{free} test set	465 reflections (5.36%)	wwPDB-VP
Wilson B-factor (Å ²)	110.8	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3529	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/925	0.47	0/1275
1	B	0.25	0/955	0.44	0/1316
2	C	0.22	0/263	0.37	0/362
2	F	0.23	0/262	0.34	0/362
3	D	0.24	0/565	0.47	0/776
3	H	0.24	0/617	0.46	0/841
All	All	0.24	0/3587	0.44	0/4932

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	909	0	757	15	0
1	B	941	0	790	18	0
2	C	256	0	191	4	0
2	F	255	0	160	1	0
3	D	559	0	501	12	0
3	H	609	0	568	15	0
All	All	3529	0	2967	57	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 57 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:51:GLU:OE1	3:H:54:ARG:NH1	2.07	0.88
1:B:130:LYS:NZ	1:B:138:THR:OG1	2.09	0.84
1:B:23:GLN:NE2	1:B:65:HIS:O	2.19	0.75
1:B:4:ILE:HD12	1:B:31:LEU:HD21	1.71	0.72
1:B:25:VAL:HG22	1:B:111:ASP:HB3	1.74	0.70

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	126/165 (76%)	123 (98%)	3 (2%)	0	100	100
1	B	131/165 (79%)	125 (95%)	6 (5%)	0	100	100
2	C	33/47 (70%)	31 (94%)	2 (6%)	0	100	100
2	F	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
3	D	78/86 (91%)	73 (94%)	5 (6%)	0	100	100
3	H	80/86 (93%)	73 (91%)	7 (9%)	0	100	100
All	All	486/596 (82%)	462 (95%)	24 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	76/150 (51%)	76 (100%)	0	100	100
1	B	80/150 (53%)	79 (99%)	1 (1%)	69	82
2	C	18/44 (41%)	18 (100%)	0	100	100
2	F	14/44 (32%)	14 (100%)	0	100	100
3	D	51/80 (64%)	50 (98%)	1 (2%)	55	76
3	H	61/80 (76%)	60 (98%)	1 (2%)	62	79
All	All	300/548 (55%)	297 (99%)	3 (1%)	76	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	LEU
3	D	21	ASP
3	H	21	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	41	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	134/165 (81%)	-0.04	3 (2%) 62 59	67, 89, 113, 129	0
1	B	139/165 (84%)	-0.12	3 (2%) 62 59	63, 86, 119, 135	0
2	C	35/47 (74%)	-0.07	2 (5%) 23 23	84, 104, 113, 118	0
2	F	40/47 (85%)	0.17	1 (2%) 57 53	99, 118, 130, 139	0
3	D	80/86 (93%)	-0.22	0 100 100	66, 91, 107, 116	0
3	H	82/86 (95%)	-0.14	1 (1%) 79 78	69, 87, 101, 105	0
All	All	510/596 (85%)	-0.09	10 (1%) 65 63	63, 90, 119, 139	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	ASP	3.1
1	A	10	ASP	2.8
3	H	-1	SER	2.7
2	C	892	TRP	2.5
1	B	41	ASP	2.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.